



wwPDB EM Validation Summary Report ⓘ

May 1, 2024 – 12:03 am BST

PDB ID : 5FYW
EMDB ID : EMD-3378
Title : Transcription initiation complex structures elucidate DNA opening (OC)
Authors : Plaschka, C.; Hantsche, M.; Dienemann, C.; Burzinski, C.; Plitzko, J.; Cramer, P.
Deposited on : 2016-03-10
Resolution : 4.35 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

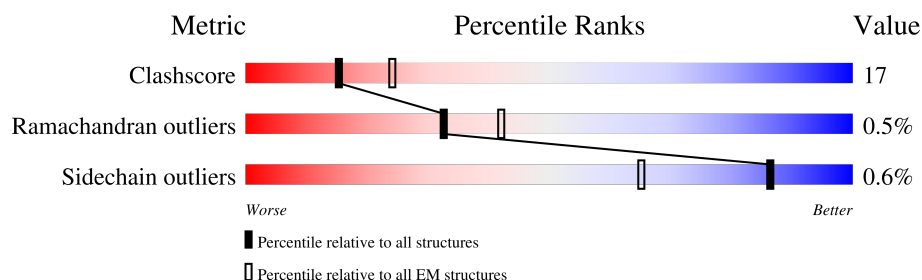
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	<div> <div>14%</div> <div>58%</div> <div>23%</div> <div>19%</div> </div>
2	B	1224	<div> <div>14%</div> <div>62%</div> <div>32%</div> <div>5%</div> </div>
3	C	318	<div> <div>52%</div> <div>31%</div> <div>18%</div> </div>
4	D	221	<div> <div>57%</div> <div>45%</div> <div>26%</div> <div>29%</div> </div>
5	E	215	<div> <div>20%</div> <div>75%</div> <div>24%</div> </div>
6	F	155	<div> <div>42%</div> <div>12%</div> <div>46%</div> </div>
7	G	171	<div> <div>49%</div> <div>51%</div> <div>48%</div> </div>
8	H	146	<div> <div>8%</div> <div>52%</div> <div>39%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	345	
14	N	72	
15	O	240	
16	Q	735	
17	R	400	
18	T	72	
19	U	286	
20	V	122	
21	W	482	
22	X	328	

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 41710 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1398	Total	C	N	O	S	0	0
			10997	6931	1927	2078	61		

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1157	Total	C	N	O	S	0	0
			9203	5822	1613	1713	55		

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	262	Total	C	N	O	S	0	0
			2061	1299	343	406	13		

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	157	Total	C	N	O	S	0	0
			1253	779	220	252	2		

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1744	1107	308	318	11		

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			670	428	114	125	3		

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	136	Total	C	N	O	S	0	0
			1089	686	184	215	4		

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			944	581	172	181	10		

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	112	Total	C	N	O	S	0	0
			904	580	154	168	2		

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

- Molecule 13 is a protein called TRANSCRIPTION INITIATION FACTOR IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	231	Total	C	N	O	S	0	0
			1785	1145	299	326	15		

- Molecule 14 is a DNA chain called NONTEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	47	Total	C	N	O	P	0	0
			919	461	178	234	46		

- Molecule 15 is a protein called TATA-BOX-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	180	Total	C	N	O	S	0	0
			1416	921	242	247	6		

- Molecule 16 is a protein called TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	148	Total	C	N	O	S	0	0
			1144	733	195	212	4		

- Molecule 17 is a protein called TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT BETA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	199	Total	C	N	O	S	0	0
			1347	838	247	255	7		

- Molecule 18 is a DNA chain called NONTEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	47	Total	C	N	O	P	0	0
			909	458	172	233	46		

- Molecule 19 is a protein called TRANSCRIPTION INITIATION FACTOR IIA LARGE SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	92	Total	C	N	O	S	0	0
			757	474	130	150	3		

- Molecule 20 is a protein called TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT

2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	100	Total	C	N	O	S	0	0
			782	492	130	156	4		

- Molecule 21 is a protein called TRANSCRIPTION INITIATION FACTOR IIE SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	168	Total	C	N	O		0	0
			835	499	168	168			

- Molecule 22 is a protein called TRANSCRIPTION INITIATION FACTOR IIE SUBUNIT BETA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	143	Total	C	N	O		0	0
			710	424	143	143			

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
23	A	2	Total	Zn	0
			2	2	
23	B	1	Total	Zn	0
			1	1	
23	C	1	Total	Zn	0
			1	1	
23	I	2	Total	Zn	0
			2	2	
23	J	1	Total	Zn	0
			1	1	
23	L	1	Total	Zn	0
			1	1	
23	M	1	Total	Zn	0
			1	1	
23	W	1	Total	Zn	0
			1	1	

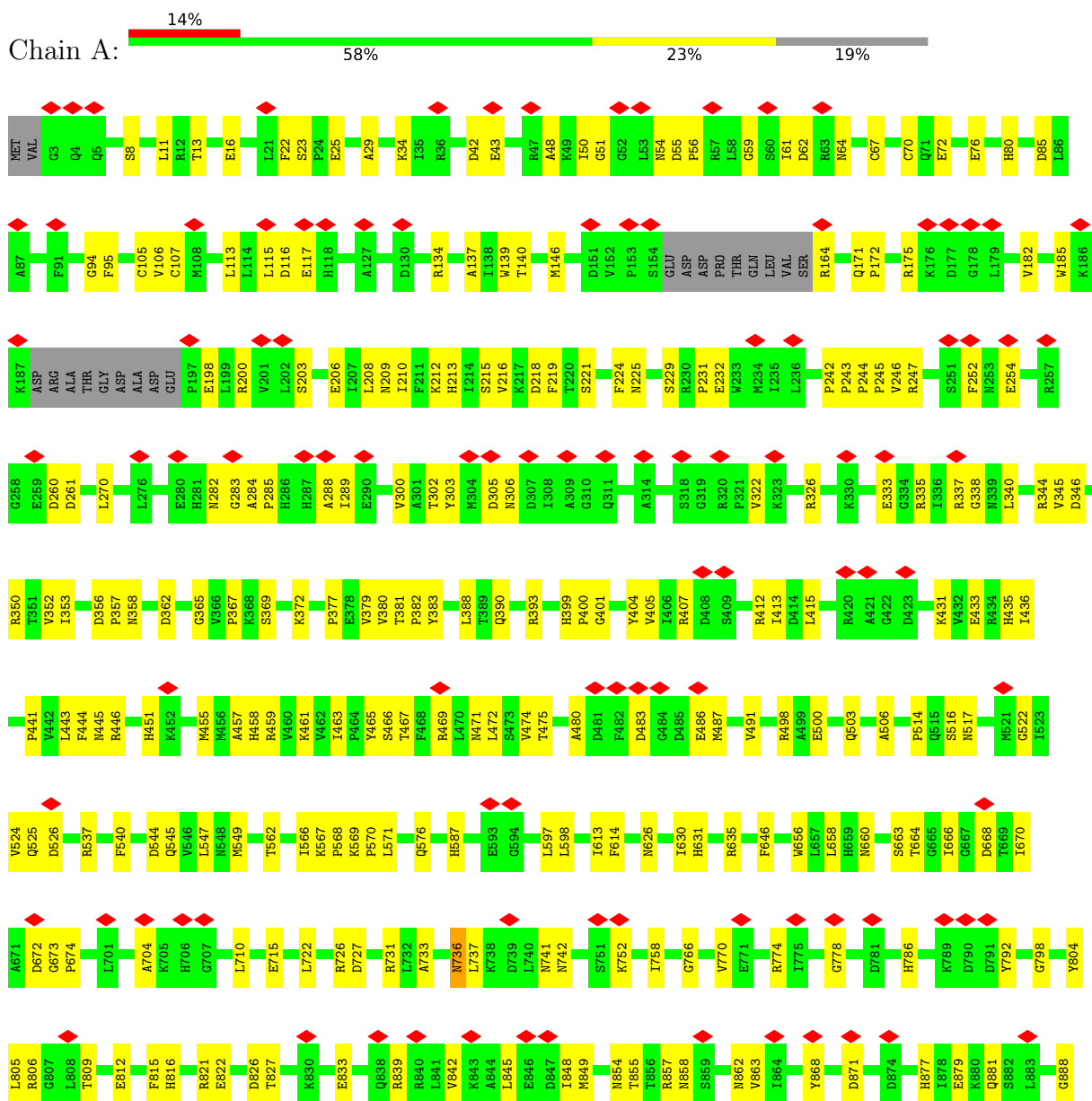
- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

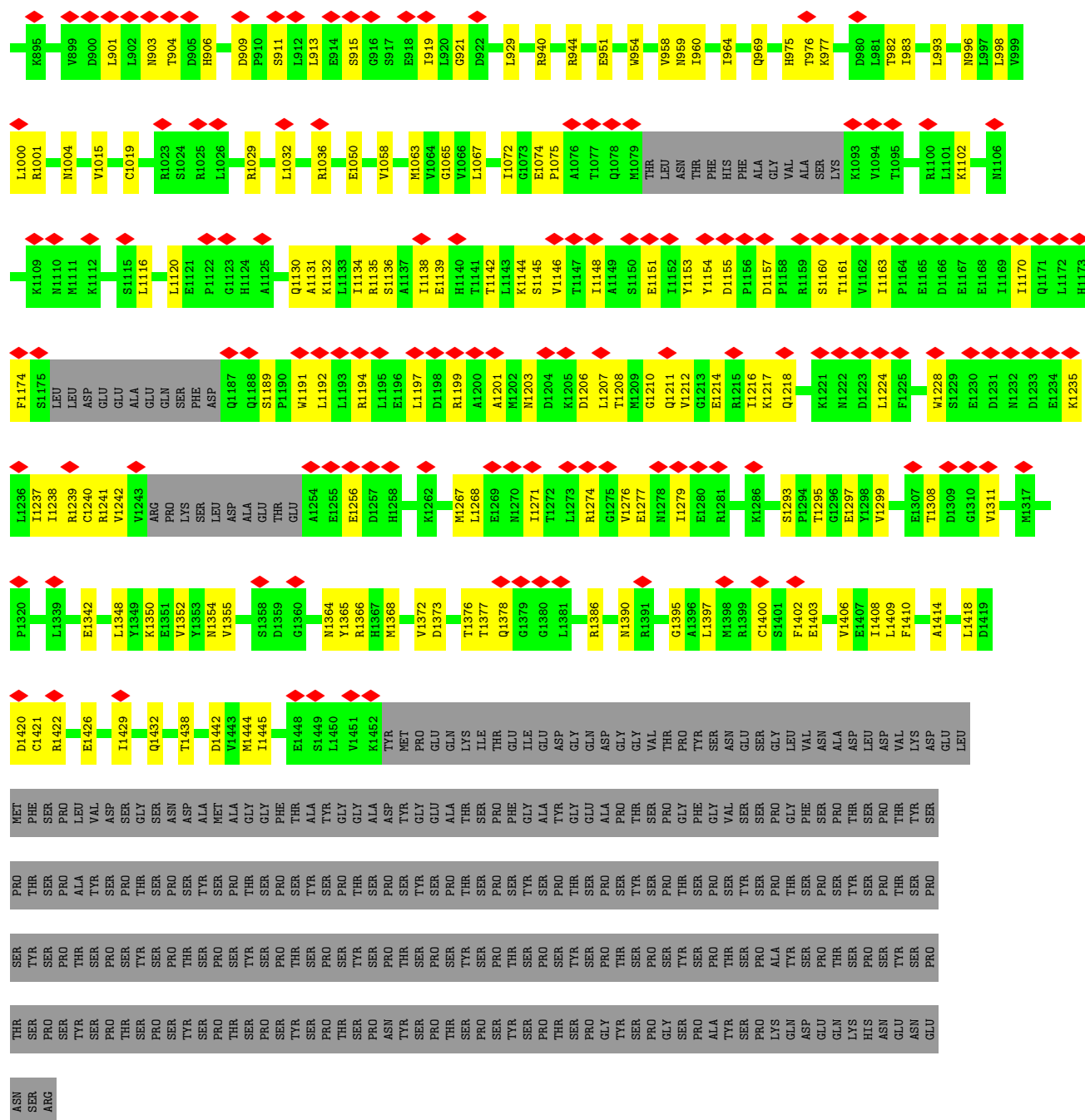
Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total	Mg	0
			1	1	

3 Residue-property plots

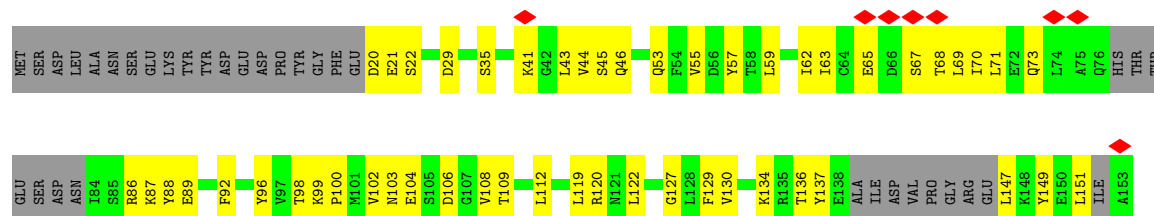
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

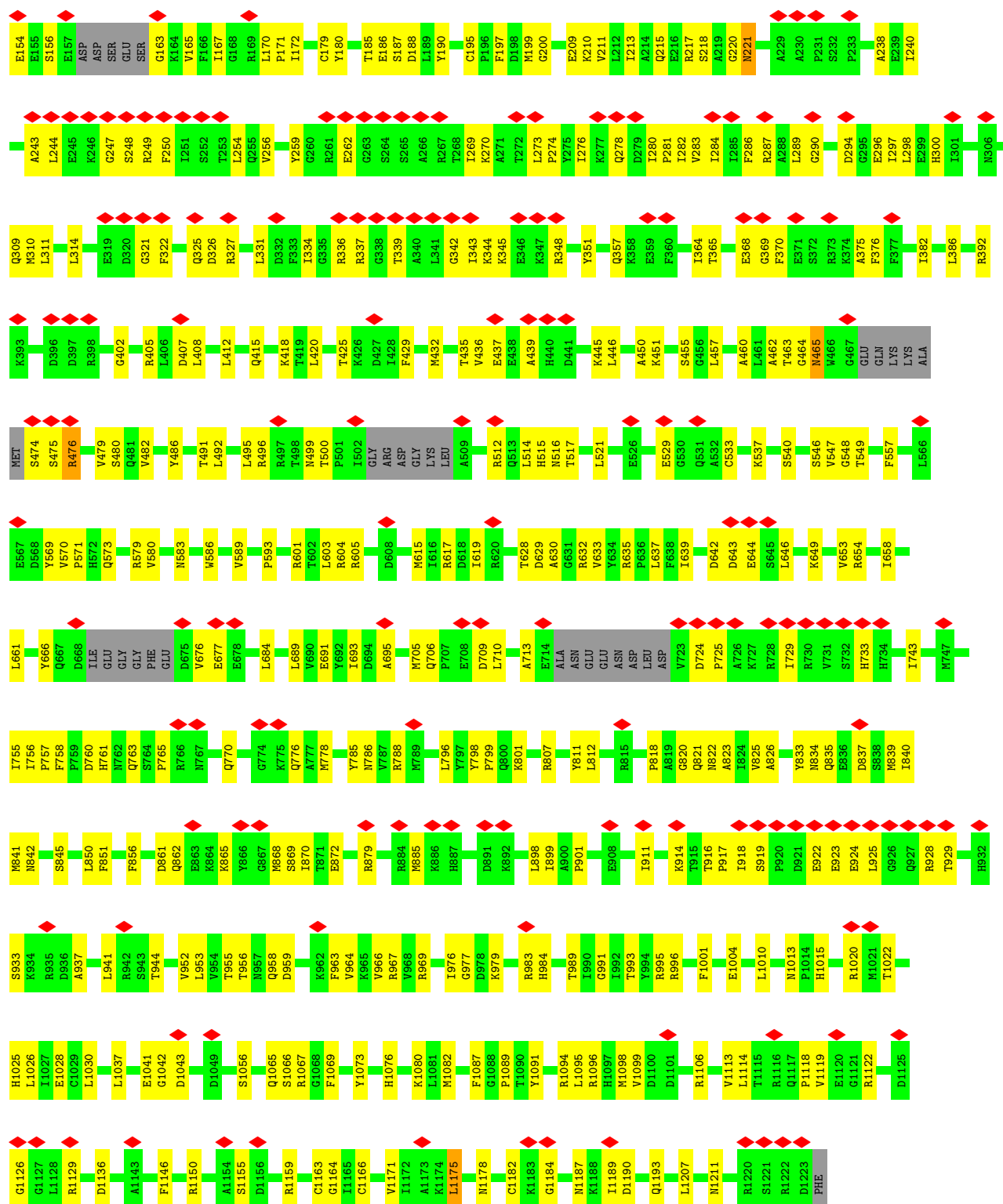
• Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1





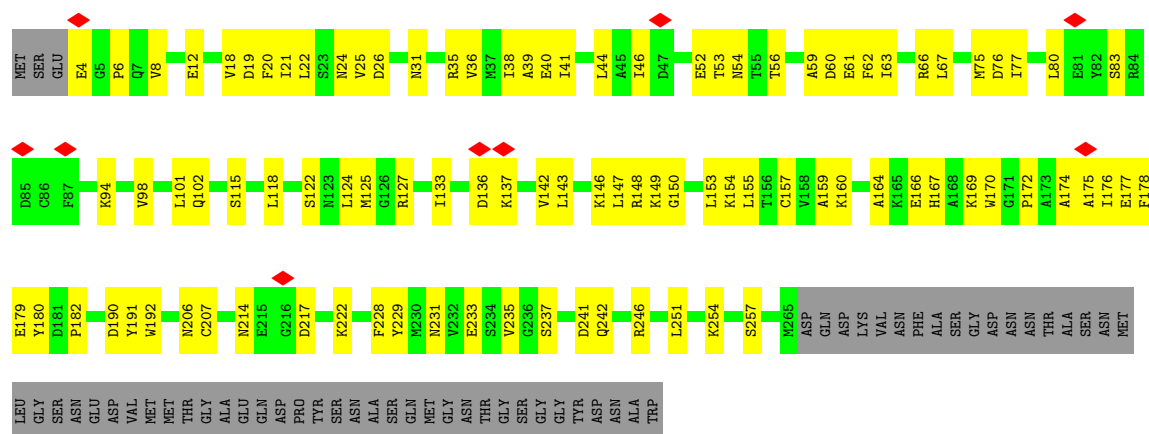
• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2



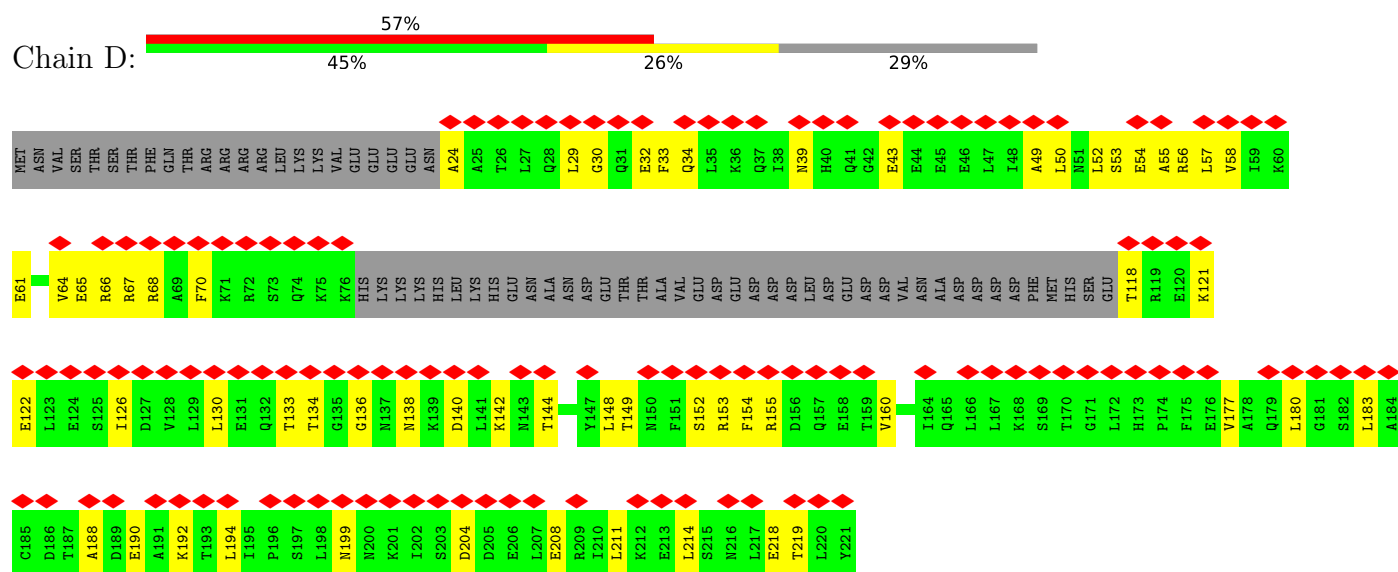


• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

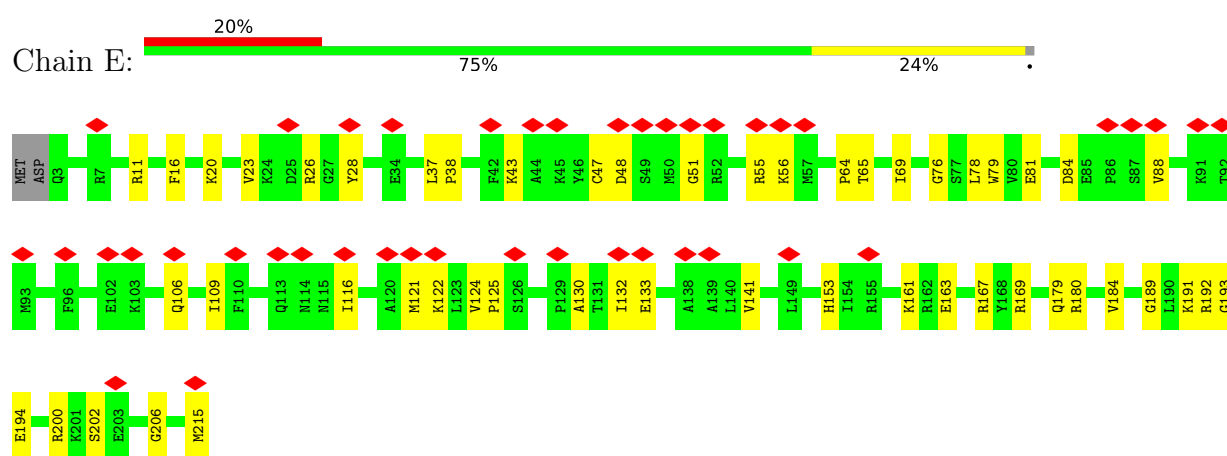




• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4



• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2



MET SER ASP THR GLU ALA PHE ASN ASP GLY ASN GLU PHE ASP PHE ASP VAL GLU HIS PHE SER ASP ASP GLU THR TVR GLU LYS GLN PHE LYS ASP ALA ASN GLY LYS THR THR ILE VAL THR GLY GLN ASP PHE GLN GLN

HIS GLU GLN ILE ARG ARG LYS THR LEU LYS K72 T82 P82 Y84 R90 A91 R92 R93 R94 L99 S102 A105 F108 V109 D110 L111 E112 V133 I134 R135 R136 Y137 D140 F143 S147 E150 D154 LEU

• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G: 49% 51% 48%

M1 F2 F3 I4 K5 D6 L7 N10 H14 P15 S16 F17 F18 R21 R22 K23 Q24 R25 L26 L31 E32 V34 E35 G36 S37 C38 K41 F42 G43 Y44 I45 L46 C47 V48 L49 D50 Y51 D52 N53 I54 D55 I56 Q57 R58 G59 R60 I61 L62 P63 T64 D65 G66 F70 Y74 V77 V78 K80 R81 F82 K83 G84 E85 V86 V87 D88 V92 S93 C94 S95 Q96 R97 F98 E99 E100 V101 Q102 V103 G104 K107 V108 F109 V110 T111 K112 H113 L114 M115 P116 Q117 D118 L119 T120 N122 A123 G124 S125 N126 P127 Y130 Q131 S132 S133 E134 D135 V136 I137 T138 I139 K140 S141 R142 R143 R144 V145 I146 I147 E148 G149 C150 I151 S152 Q153 V154 S155 S156 I157 H158 A159 I160 G161 S162 T163 K164 E165 D166 Y167 L168 G169 A170 I171

• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H: 8% 52% 39% 7%

MET S2 N3 T4 L5 F6 D7 D8 I9 F10 S13 K22 V23 C24 R25 I26 E27 S30 D34 Q35 C36 D41 I42 M43 V44 E45 L46 T56 A60 S61 N64 L65 Q137 E138 N139 L143 I144 R145 R146 A90 D91 D92 Y93 D94 Y95 V96 T100 A101 Y102 K103 F104 E105 E106 V107 S108 K109 D110 L111 I112 Y115 Y116 S117 G120 L121 L122 M123 R124 L125 E126 Y129 R130 N131 L132 N133 K136 Q137 E138 N139 L143 I144 R145 R146

• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

Chain I: 51% 61% 34% 5%

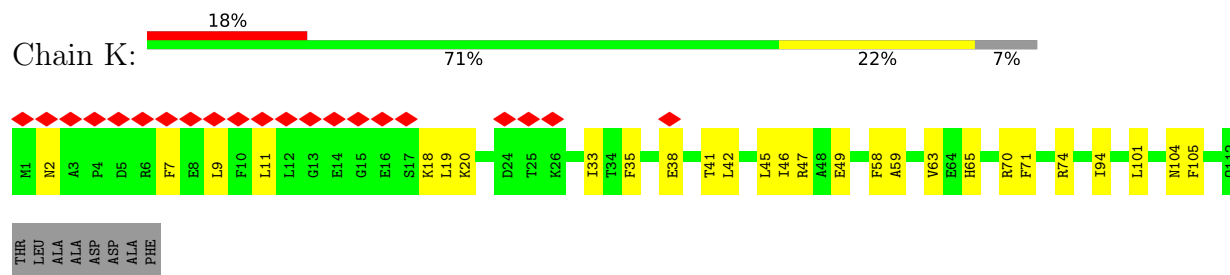
MET T2 T3 F4 R5 F6 C7 R8 D9 M13 L14 R17 E18 D19 K20 E21 N22 N23 R24 R25 L26 F27 E28 T31 C32 S33 Y34 V35 E36 E37 A38 G39 S40 P41 L42 V43 Y44 R45 H46 E47 L48 I49 T50 N51 I52 G53 E54 T55 A56 G57 V58 V59 Q60 D61 I62 G63 S64 D65 P66 T67 R70 S71 E74 K77 H79 S80 R81 E82 N83 V84 Q87 S88 Q89 R90 R91 R92 K93 D94 T95 S96 F100 F101 Y102 C103 S105 C106 S107 H108 I109 S112 D113 Q114 K115 N116 K117 ARG THR GLN PHE SER

• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

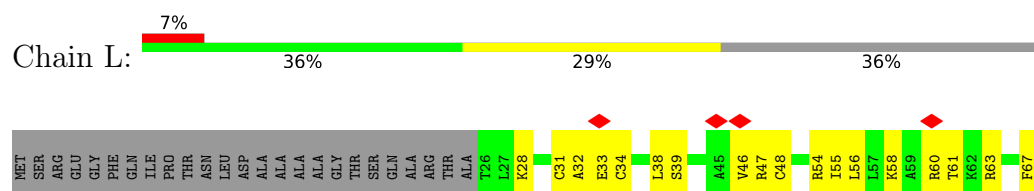
Chain J: 7% 64% 27% 7%

M1 I2 R6 C7 F8 V13 D16 K17 W18 Y21 L25 Q26 E27 D28 E29 L30 T34 R38 L39 G40 L41 K42 R43 Y44 C45 C46 R47 R48 T52 E58 M64 P65 LEU GLU LYS ARG ASP

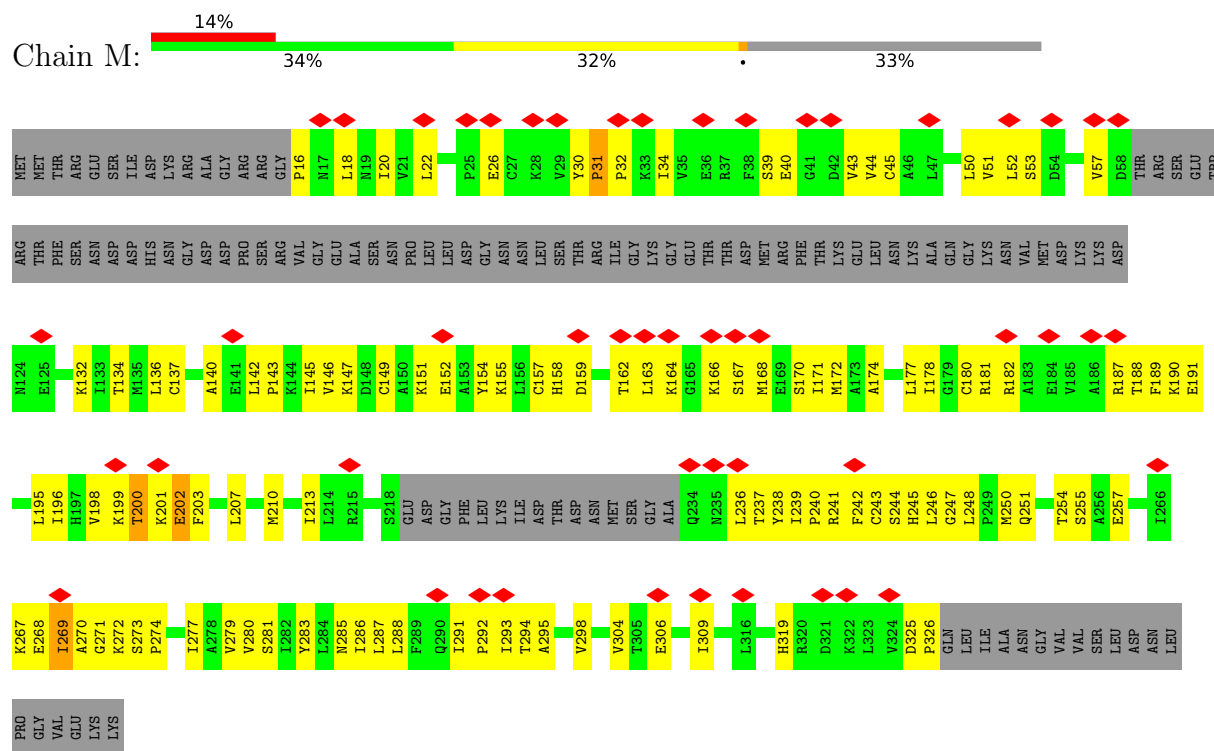
- Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11



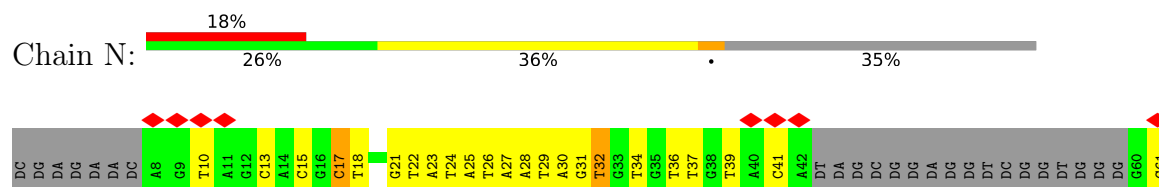
- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4



- Molecule 13: TRANSCRIPTION INITIATION FACTOR IIB

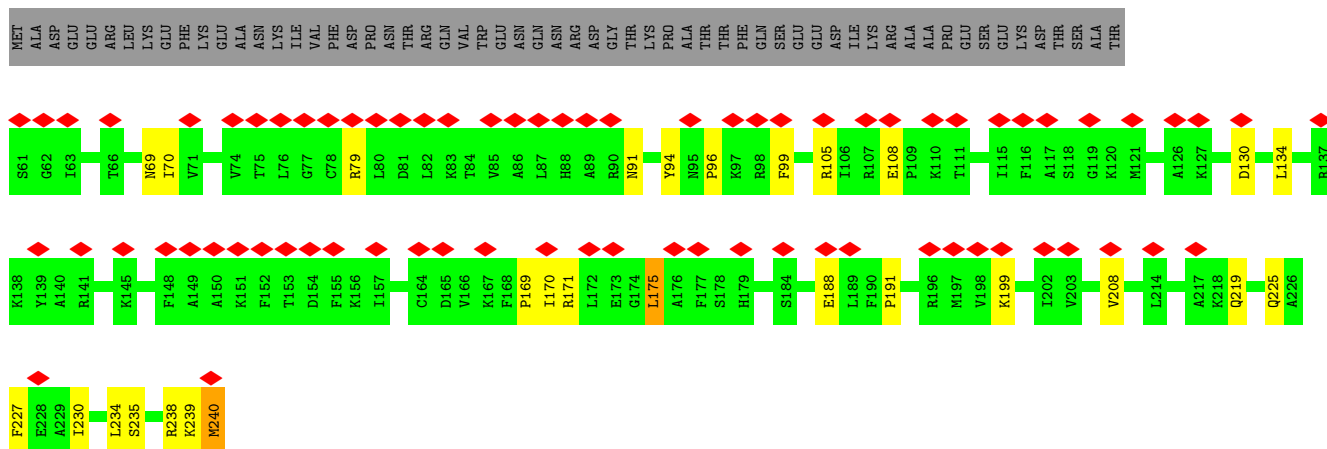


- Molecule 14: NONTEMPLATE DNA

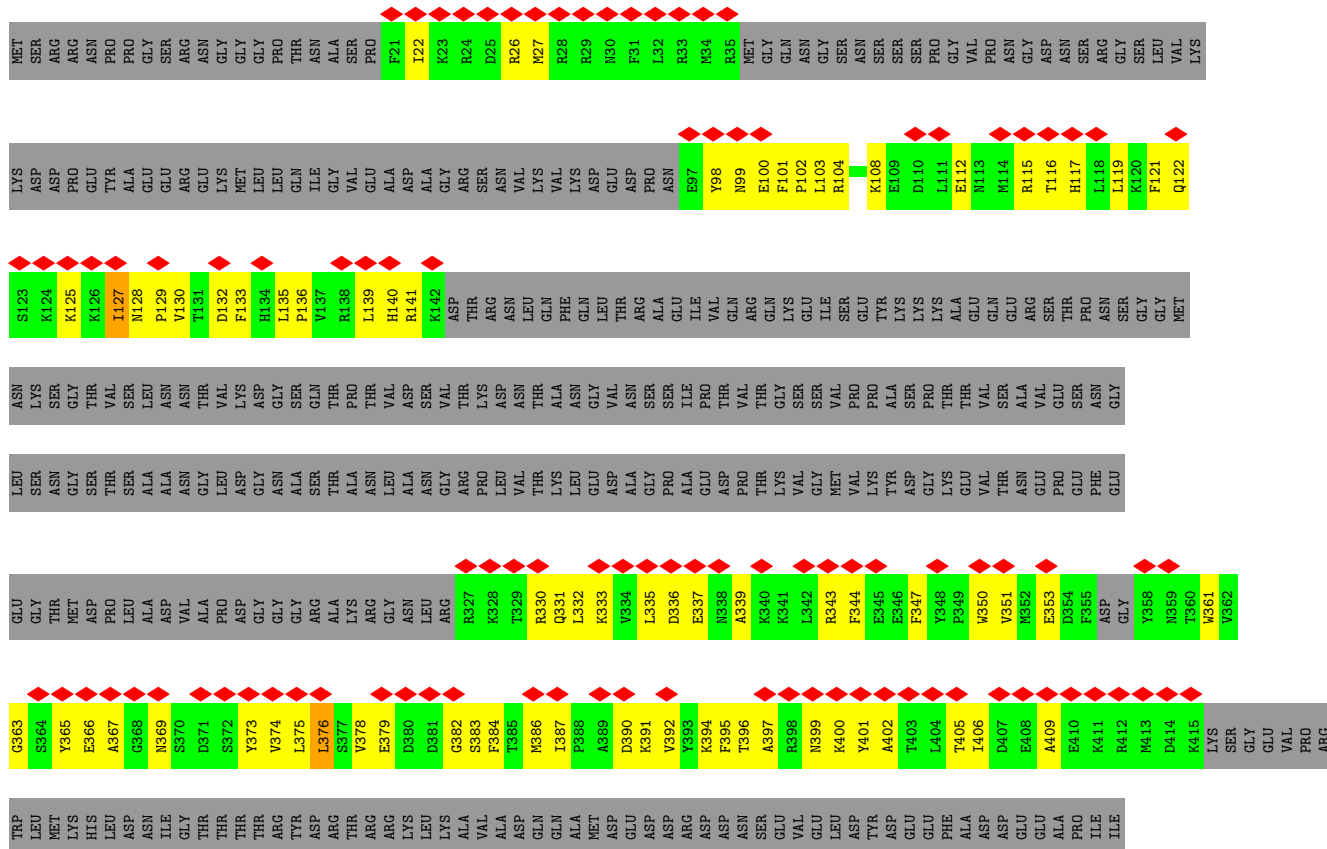


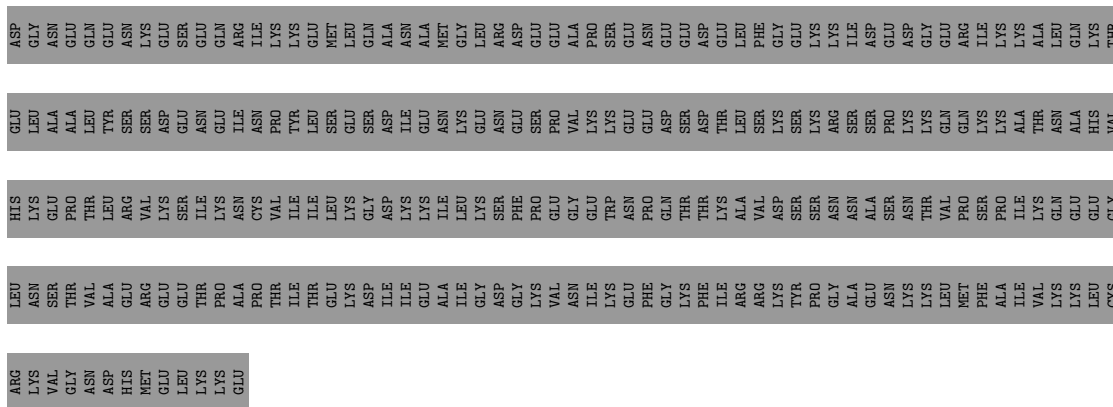


Chain O:  31% 63% 11% 25%

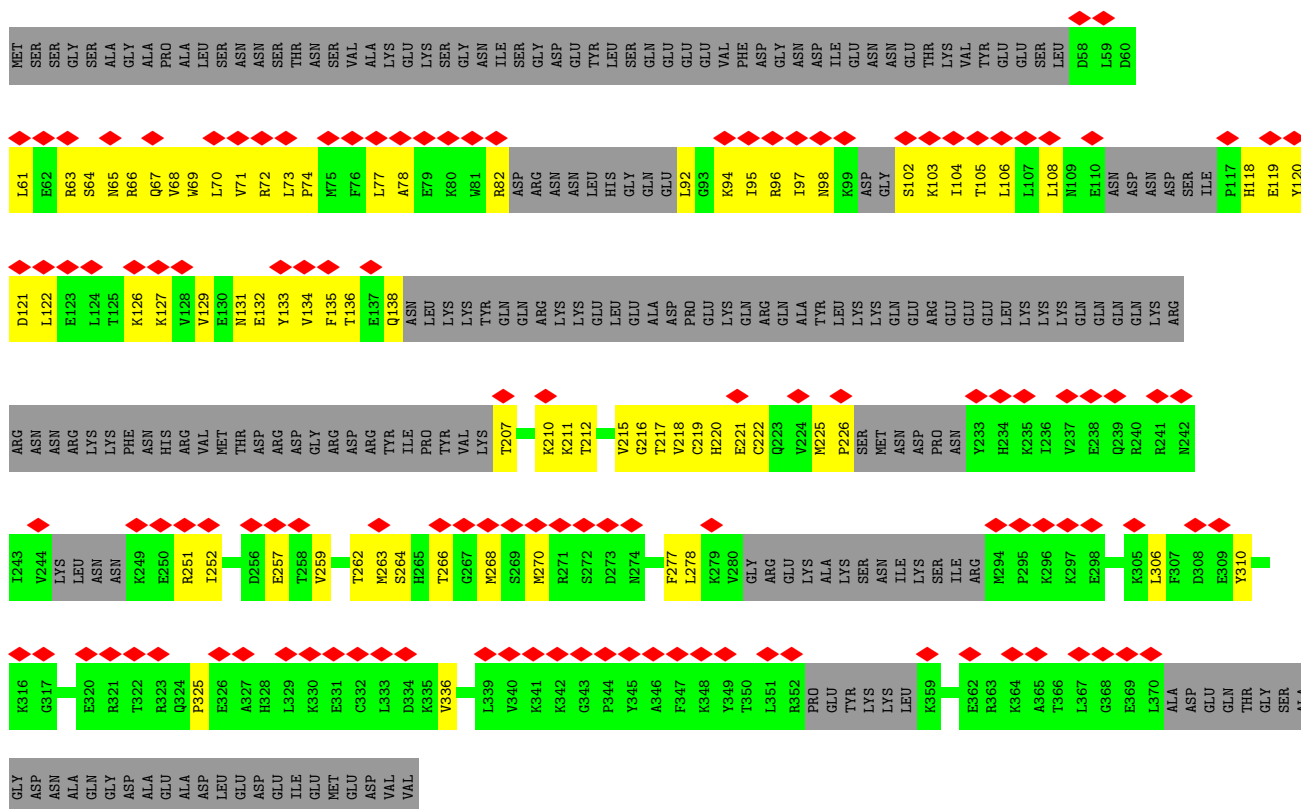
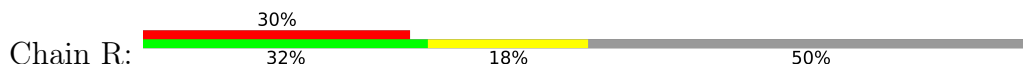


Chain Q:  10% 10% 13% 80%

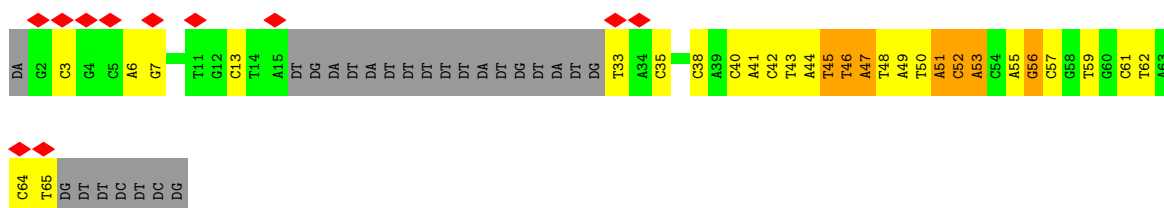
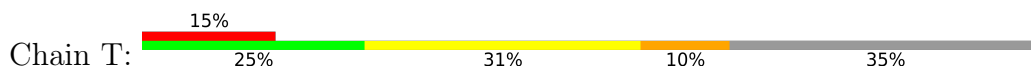




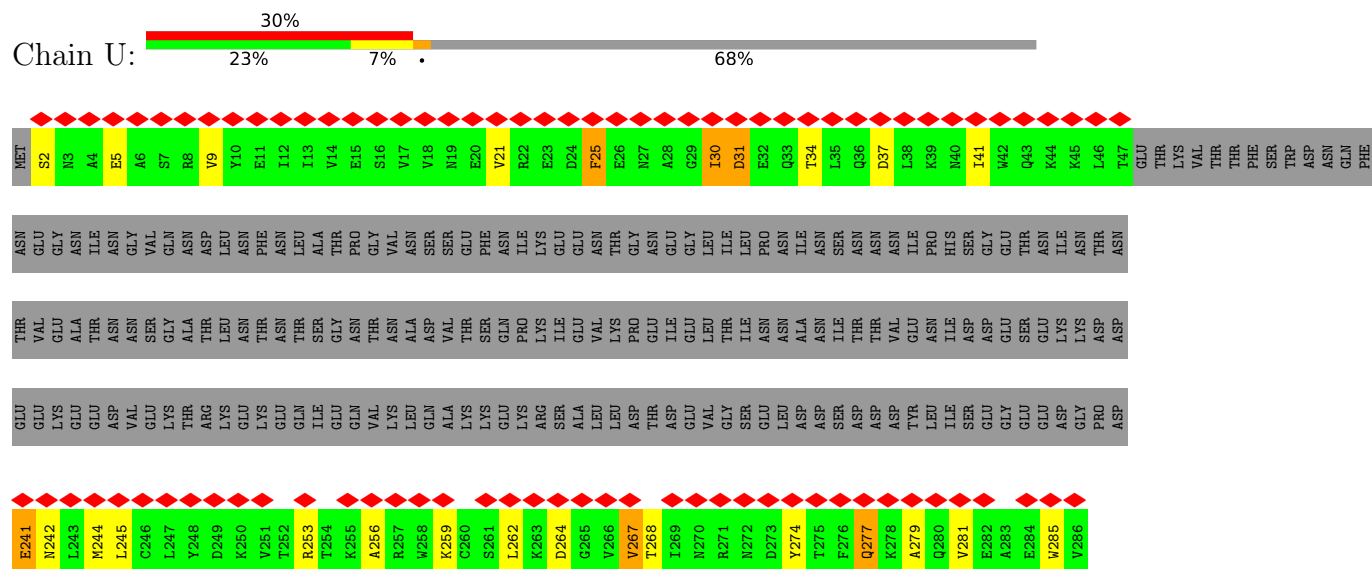
● Molecule 17: TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT BETA



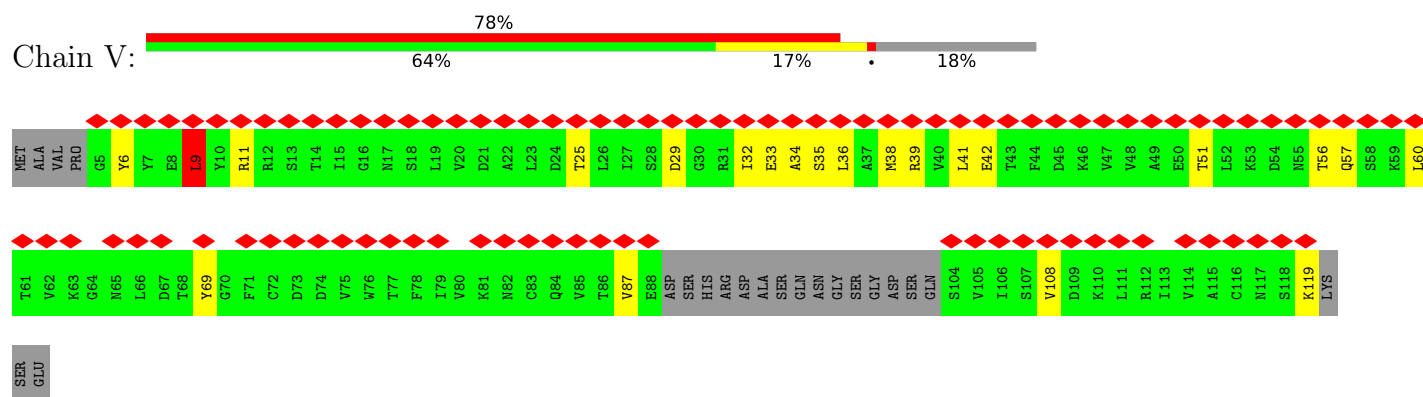
- Molecule 18: NONTEMPLATE DNA



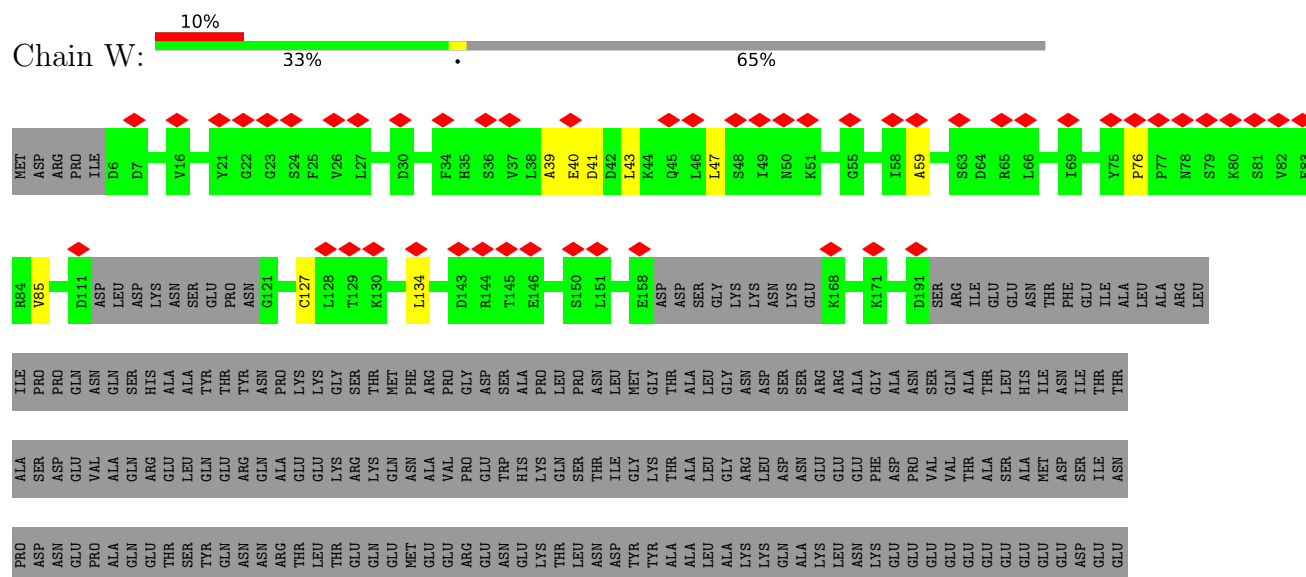
• Molecule 19: TRANSCRIPTION INITIATION FACTOR IIA LARGE SUBUNIT



• Molecule 20: TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT 2



• Molecule 21: TRANSCRIPTION INITIATION FACTOR IIE SUBUNIT ALPHA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	11231	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	33	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	4200	Depositor
Magnification	37037	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	-0.039	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0325	Depositor
Map size (\AA)	405.0, 405.0, 405.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.35, 1.35, 1.35	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.46	0/11192	0.55	1/15128 (0.0%)
2	B	0.51	0/9381	0.59	1/12650 (0.0%)
3	C	0.52	0/2099	0.57	0/2845
4	D	0.25	0/1262	0.44	0/1693
5	E	0.40	0/1780	0.49	0/2395
6	F	0.47	0/682	0.52	0/922
7	G	0.31	0/1368	0.50	0/1844
8	H	0.61	1/1107 (0.1%)	0.97	6/1499 (0.4%)
9	I	0.40	0/962	0.50	0/1295
10	J	0.53	0/541	0.56	0/727
11	K	0.43	0/922	0.53	0/1244
12	L	0.40	0/360	0.60	0/478
13	M	0.40	0/1809	0.60	0/2435
14	N	1.07	12/1036 (1.2%)	1.30	5/1530 (0.3%)
15	O	0.59	0/1443	0.78	1/1942 (0.1%)
16	Q	0.53	0/1168	0.68	1/1579 (0.1%)
17	R	0.43	0/1354	0.68	1/1832 (0.1%)
18	T	1.24	16/1023 (1.6%)	1.44	13/1507 (0.9%)
19	U	0.39	0/766	0.61	0/1032
20	V	0.38	0/789	0.62	1/1066 (0.1%)
21	W	0.33	1/832 (0.1%)	0.47	0/1157
22	X	0.26	0/706	0.47	0/979
All	All	0.52	30/42582 (0.1%)	0.65	30/57779 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	2
10	J	0	1
13	M	0	1
All	All	0	5

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	131	ASN	C-N	-13.08	1.03	1.34
18	T	53	DA	P-O5'	-11.50	1.48	1.59
18	T	47	DA	C1'-N9	-10.28	1.32	1.47
18	T	56	DG	C1'-N9	-6.75	1.37	1.47
18	T	64	DC	C1'-N1	6.24	1.57	1.49

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	131	ASN	N-CA-C	16.18	154.67	111.00
8	H	131	ASN	O-C-N	-15.85	97.34	122.70
8	H	131	ASN	C-N-CA	15.68	160.91	121.70
18	T	46	DT	O4'-C4'-C3'	-11.75	98.95	106.00
17	R	336	VAL	CB-CA-C	-10.95	90.60	111.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1175	LEU	Peptide
8	H	131	ASN	Peptide,Mainchain
10	J	2	ILE	Peptide
13	M	292	PRO	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10997	0	11082	291	0
2	B	9203	0	9203	371	0
3	C	2061	0	2029	72	0
4	D	1253	0	1273	62	0
5	E	1744	0	1772	32	0
6	F	670	0	690	15	0
7	G	1340	0	1356	95	0
8	H	1089	0	1061	40	0
9	I	944	0	899	30	0
10	J	532	0	543	22	0
11	K	904	0	911	20	0
12	L	358	0	380	24	0
13	M	1785	0	1891	170	0
14	N	919	0	533	33	0
15	O	1416	0	1493	69	0
16	Q	1144	0	1034	100	0
17	R	1347	0	1130	92	0
18	T	909	0	533	65	0
19	U	757	0	747	21	0
20	V	782	0	790	16	0
21	W	835	0	349	12	0
22	X	710	0	287	4	0
23	A	2	0	0	0	0
23	B	1	0	0	0	0
23	C	1	0	0	0	0
23	I	2	0	0	0	0
23	J	1	0	0	0	0
23	L	1	0	0	0	0
23	M	1	0	0	0	0
23	W	1	0	0	0	0
24	A	1	0	0	0	0
All	All	41710	0	39986	1351	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 1351 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:865:LYS:CE	13:M:145:ILE:HD11	1.46	1.44
2:B:405:ARG:NH1	2:B:632:ARG:HG2	1.23	1.40
2:B:868:MET:HB2	13:M:149:CYS:SG	1.64	1.35
13:M:267:LYS:HE3	15:O:208:VAL:CG1	1.59	1.31
13:M:272:LYS:HB3	18:T:53:DA:P	1.71	1.29

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1386/1733 (80%)	1306 (94%)	77 (6%)	3 (0%)	47	81
2	B	1139/1224 (93%)	1086 (95%)	48 (4%)	5 (0%)	34	72
3	C	260/318 (82%)	246 (95%)	14 (5%)	0	100	100
4	D	153/221 (69%)	145 (95%)	8 (5%)	0	100	100
5	E	211/215 (98%)	209 (99%)	2 (1%)	0	100	100
6	F	81/155 (52%)	76 (94%)	5 (6%)	0	100	100
7	G	169/171 (99%)	160 (95%)	8 (5%)	1 (1%)	25	65
8	H	132/146 (90%)	114 (86%)	14 (11%)	4 (3%)	4	32
9	I	114/122 (93%)	105 (92%)	9 (8%)	0	100	100
10	J	63/70 (90%)	57 (90%)	5 (8%)	1 (2%)	9	45
11	K	110/120 (92%)	107 (97%)	3 (3%)	0	100	100
12	L	43/70 (61%)	37 (86%)	6 (14%)	0	100	100
13	M	225/345 (65%)	202 (90%)	20 (9%)	3 (1%)	12	48
15	O	178/240 (74%)	174 (98%)	4 (2%)	0	100	100
16	Q	140/735 (19%)	124 (89%)	13 (9%)	3 (2%)	7	39
17	R	181/400 (45%)	171 (94%)	9 (5%)	1 (1%)	25	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	U	88/286 (31%)	82 (93%)	3 (3%)	3 (3%)	3	29
20	V	96/122 (79%)	87 (91%)	8 (8%)	1 (1%)	15	54
21	W	162/482 (34%)	154 (95%)	7 (4%)	1 (1%)	25	65
22	X	135/328 (41%)	125 (93%)	9 (7%)	1 (1%)	22	62
All	All	5066/7503 (68%)	4767 (94%)	272 (5%)	27 (0%)	32	68

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	343	ILE
2	B	476	ARG
8	H	132	LEU
13	M	269	ILE
17	R	259	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1221/1520 (80%)	1219 (100%)	2 (0%)	93	96
2	B	1000/1061 (94%)	999 (100%)	1 (0%)	93	97
3	C	230/274 (84%)	230 (100%)	0	100	100
4	D	139/200 (70%)	139 (100%)	0	100	100
5	E	195/197 (99%)	195 (100%)	0	100	100
6	F	73/137 (53%)	73 (100%)	0	100	100
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	119/128 (93%)	119 (100%)	0	100	100
9	I	110/116 (95%)	110 (100%)	0	100	100
10	J	60/65 (92%)	60 (100%)	0	100	100
11	K	97/102 (95%)	97 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	201/299 (67%)	200 (100%)	1 (0%)	88	93
15	O	152/205 (74%)	141 (93%)	11 (7%)	14	41
16	Q	109/641 (17%)	109 (100%)	0	100	100
17	R	107/363 (30%)	107 (100%)	0	100	100
19	U	84/260 (32%)	79 (94%)	5 (6%)	19	46
20	V	90/108 (83%)	85 (94%)	5 (6%)	21	48
All	All	4179/5885 (71%)	4154 (99%)	25 (1%)	86	92

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	O	240	MET
19	U	253	ARG
20	V	108	VAL
19	U	241	GLU
19	U	267	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
15	O	219	GLN
16	Q	122	GLN
20	V	57	GLN
19	U	280	GLN
4	D	143	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	131:ASN	C	132:LEU	N	1.04

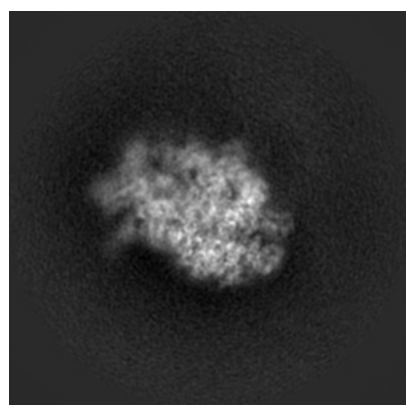
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3378. These allow visual inspection of the internal detail of the map and identification of artifacts.

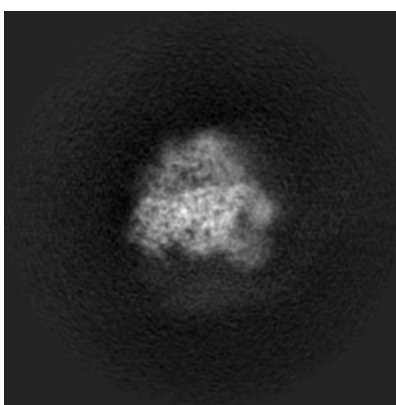
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

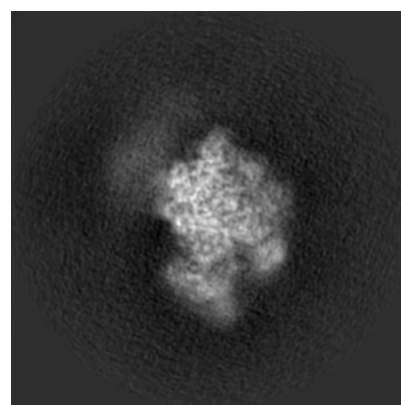
6.1.1 Primary map



X



Y

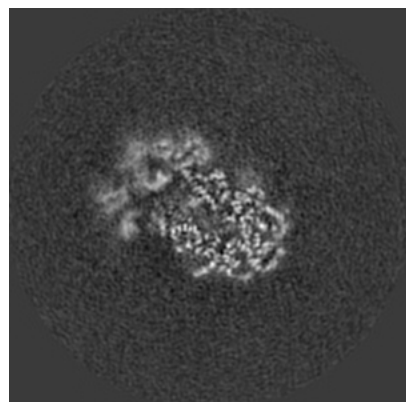


Z

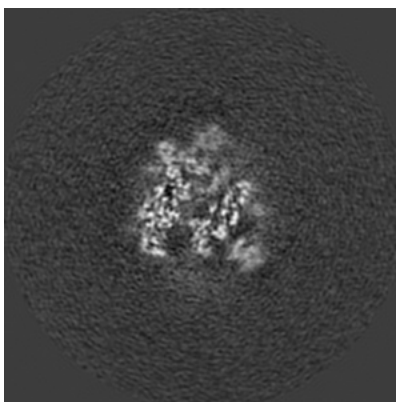
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

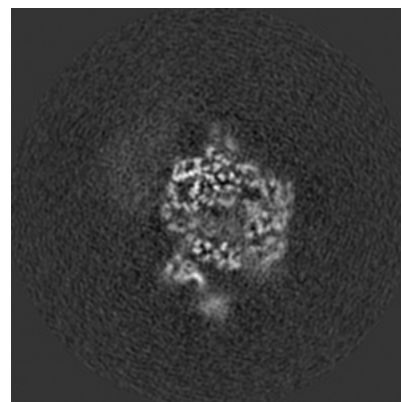
6.2.1 Primary map



X Index: 150



Y Index: 150

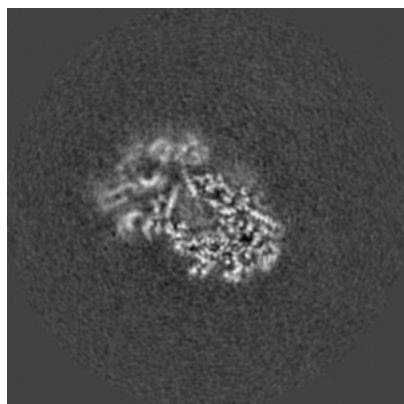


Z Index: 150

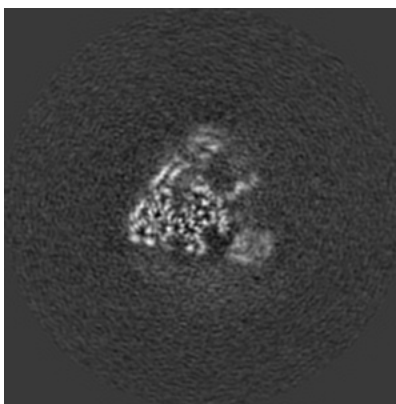
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

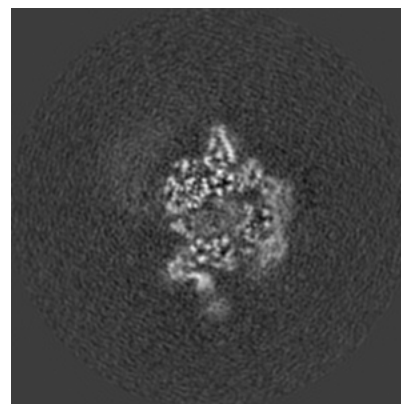
6.3.1 Primary map



X Index: 146



Y Index: 165

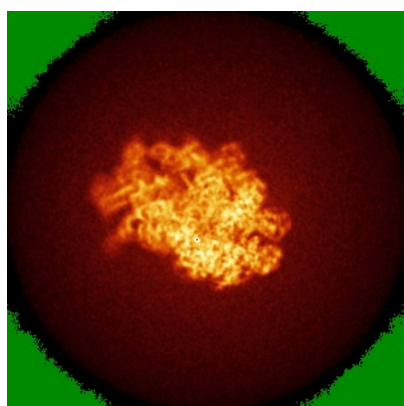


Z Index: 146

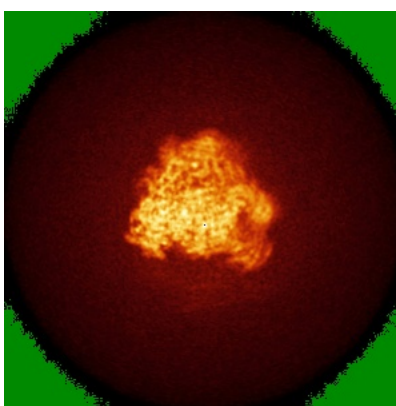
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

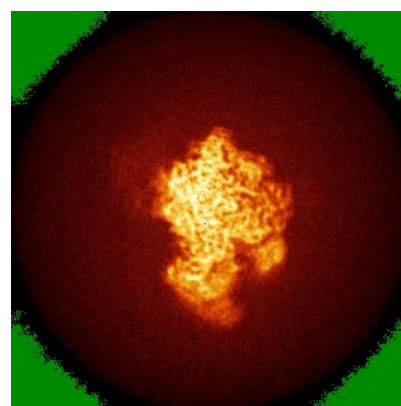
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0325. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

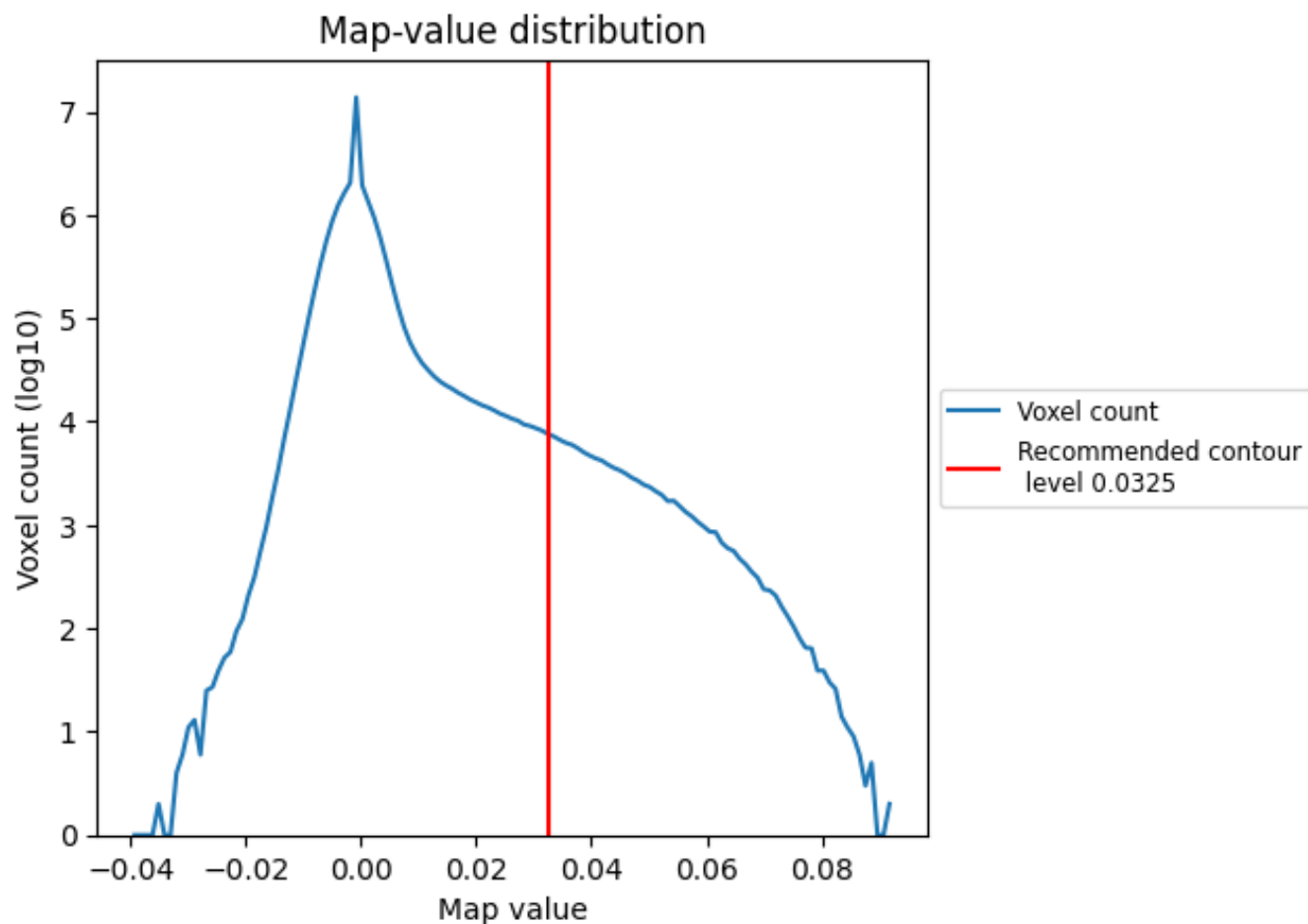
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

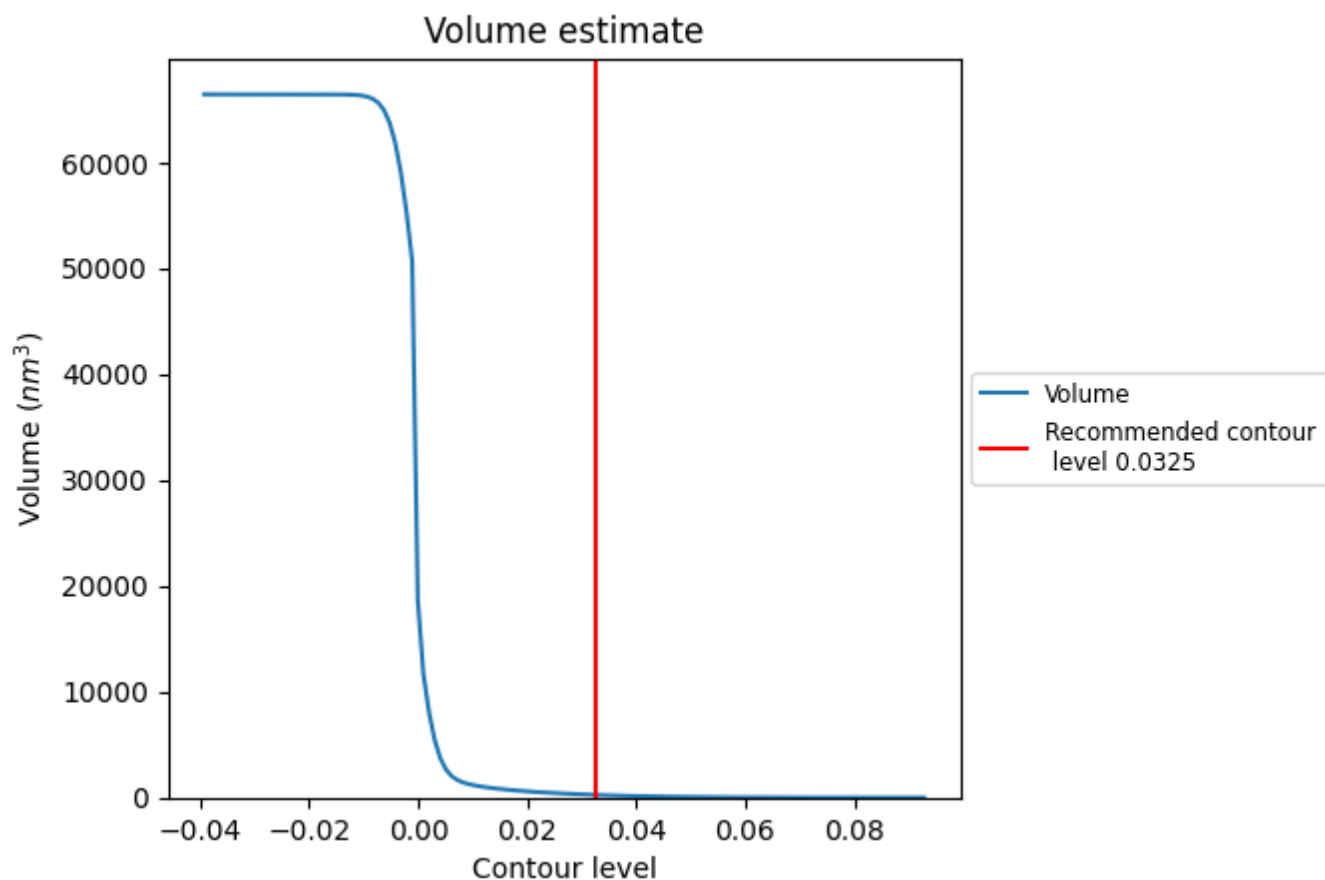
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

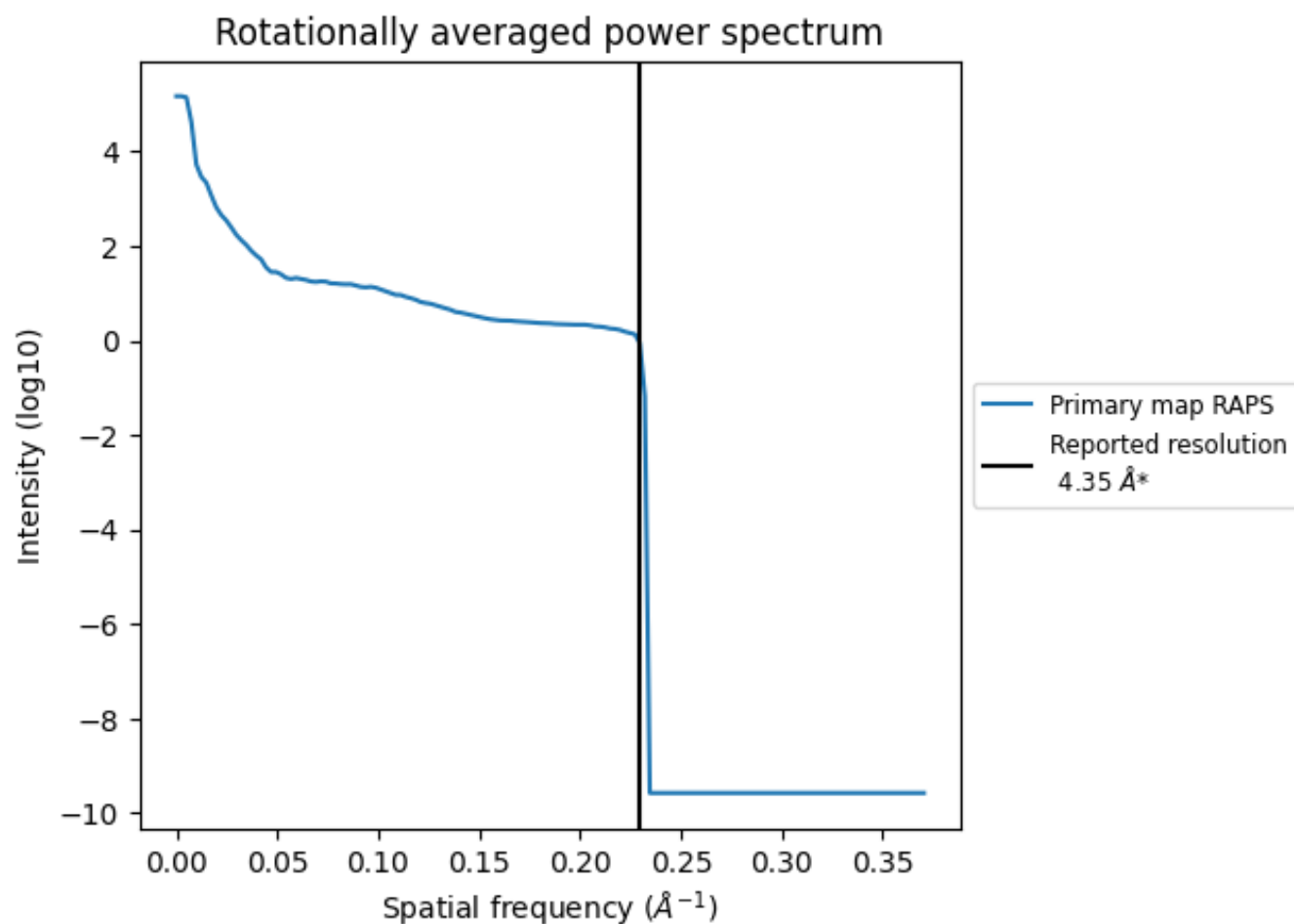
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 250 nm³; this corresponds to an approximate mass of 226 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.230 \AA^{-1}

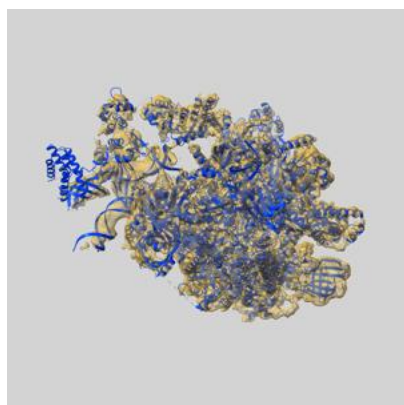
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

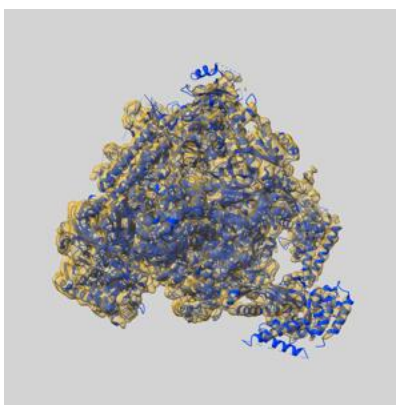
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3378 and PDB model 5FYW. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

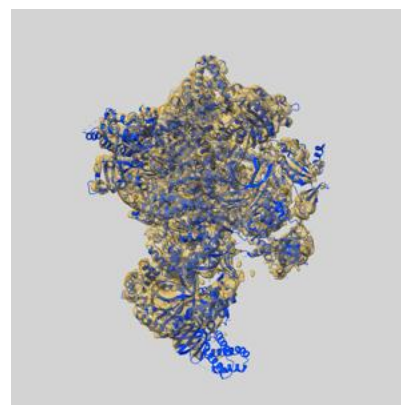
9.1 Map-model overlay [i](#)



X



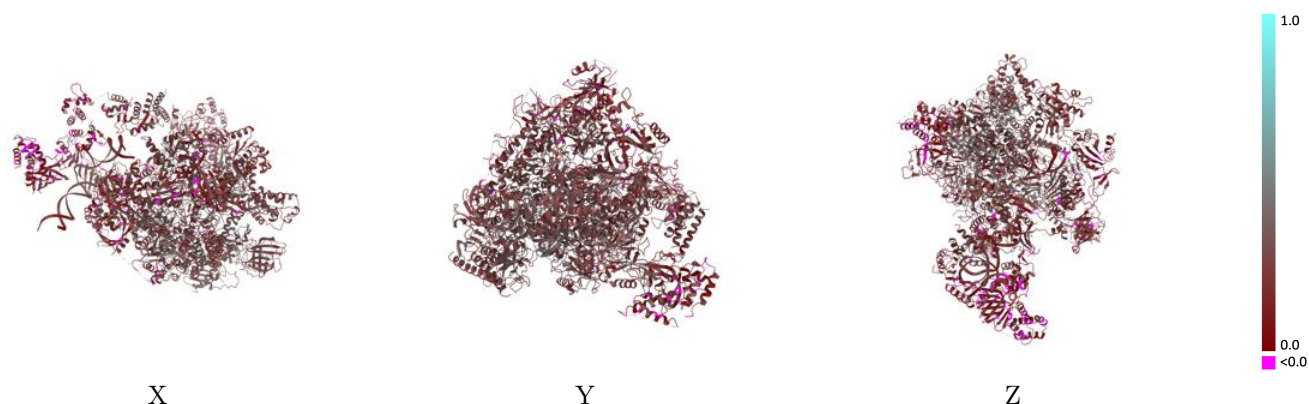
Y



Z

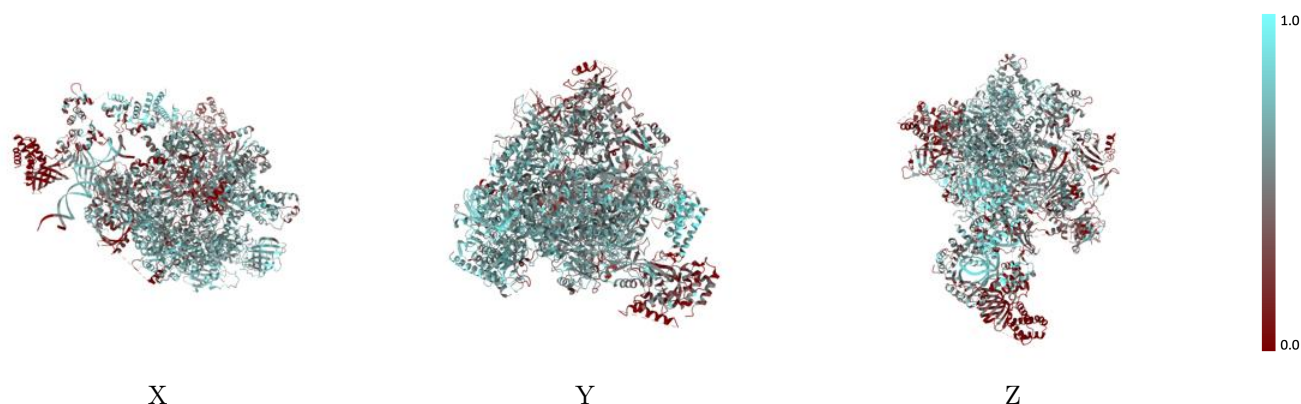
The images above show the 3D surface view of the map at the recommended contour level 0.0325 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



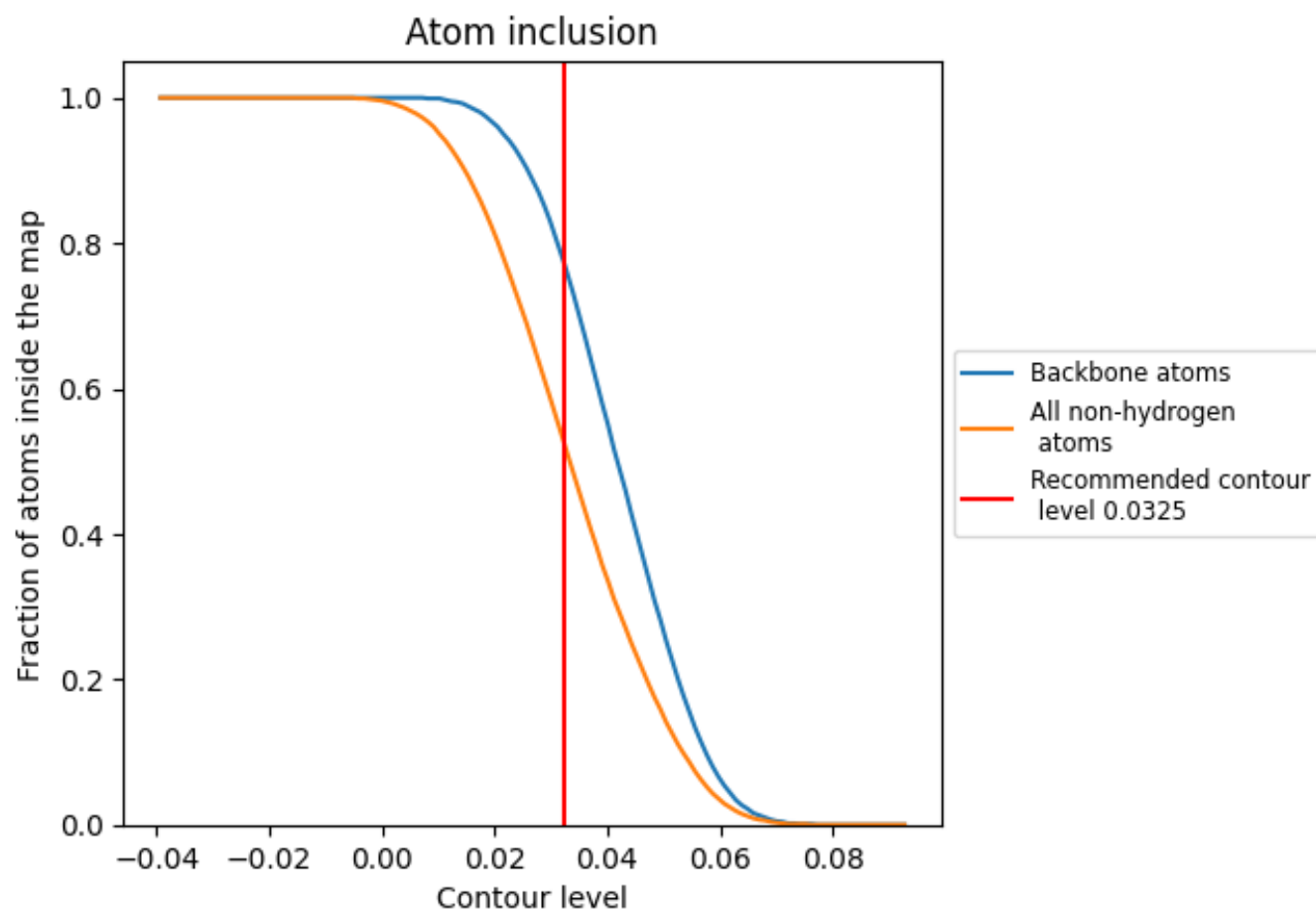
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0325).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 52% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0325) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5210	 0.2600
A	 0.5660	 0.2900
B	 0.5770	 0.3040
C	 0.6790	 0.3190
D	 0.1920	 0.1420
E	 0.5400	 0.2590
F	 0.6170	 0.2990
G	 0.3910	 0.2230
H	 0.6470	 0.2980
I	 0.3760	 0.2100
J	 0.6690	 0.3070
K	 0.5470	 0.2990
L	 0.6160	 0.3150
M	 0.5350	 0.2430
N	 0.5680	 0.2020
O	 0.4430	 0.1560
Q	 0.3080	 0.1880
R	 0.3630	 0.2010
T	 0.5970	 0.1930
U	 0.0890	 0.0950
V	 0.0930	 0.1140
W	 0.6520	 0.2270
X	 0.5030	 0.1730

